Project H-5: Research of new X-TM-Y alloys (X=Ca, Mg, Li; TM=transition metals, Y=metals)

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1. Objective

The objective of this project is to search for the new intermetallic compounds and alloys with the possibility of large hydrogen storage capacities. This project is exploratory and limited to a preliminary experimental survey on possibilities for gaseous hydrogen storage.

2. Latest results

In 2002 we confirmed that a new ternary hydride was formed through the decomposition of hydrogenated $CaNi_2$ and $CaNi_3$ alloys in H_2 atmospheres. The new hydride had the CsCl type structure for its constituent metal atoms and its hydrogen storage capacity was 1.5H/M (H/M: molar ratio of hydrogen to metal). In the case that the hydride is prepared through the decomposition of $CaNi_2$ or $CaNi_3$ hydrides, it is impossible to obtain a $CaNiH_3$ sample with the single phase structure; the sample so obtained contains a secondary phase such as metallic nickel. In 2003, we tried to prepare the $CaNiH_3$ sample with single phase structure.

Firstly we tried to prepare the target sample by a sintering method. CaH_2 and metallic nickel were chosen as starting materials and they were weighed so that the nominal compositional ratio of Ca to Ni could be 1, mixed and then cold-pressed under a purified argon atmosphere. The pellet was put into Al_2O_3 crucible and then heated at 673K in an H_2 atmosphere of 0.7MPa for 24 hours. The reaction of CaH_2 with metallic nickel was not observed under those conditions.

Next, mechanical grinding was applied to prepare the target sample. In this case, the alloy with the bulk composition of Ca:Ni=1:0.96, which has a multiphase structure composed of Ca, $CaNi_2$ and $CaNi_3$, was chosen as a starting material. The starting material was mechanically ground in an H_2 atmosphere of 0.7MPa for 3-40 hours. The X-ray diffraction profile of the sample milled for 3 hours exhibited that its original constituent phases changed to their corresponding hydride ones. However the X-ray diffraction profile of the sample milled for 40 hours exhibited the formation of $CaNiH_3$, although there existed small amounts of minor phases such as metallic nickel.

3. Future work

Since it was found that the sample with a single phase structure composed of $CaNiH_3$ can be prepared by mechanical grinding, structural analysis such as neutron diffraction will be applied to the so prepared sample in order to obtain the detailed information about the $CaNiH_3$. The rehydrogenation of the sample after decomposition in H_2 atmosphere will be tried in order to find the way that $CaNiH_3$ can reversibly absorb and desorb hydrogen. In addition, the effect of the additives on the improvement of the stability of the hydride will be examined.